

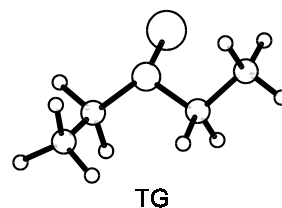
1805 C₄H₁₀ClNED, *ab initio* calculations

(HF/3-3-21G* (for C, N, H)

HF/4-21G* (for Cl))

***N*-Chloro-*N*-ethylethanamine**C_s (TT)C₁ (TG)

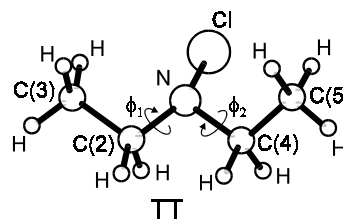
r_g	Å ^{a)}	θ_α	deg ^{a)}
N-C	1.471(2)	N-C-C	112.6(4)
N-Cl	1.765(2)	N-C-H (mean)	109.6(18)
C-C	1.530(3)	C-N-C	110.6(8)
C-H (mean)	1.118(3)	C-N-Cl	108.3(2)
		C-C-H (mean)	109.4(11)
		ϕ_1 ^{b)} = $(-\phi_2)$ ^{c)}	175(1)



The molecule exists as a mixture of TT and TG (dihedral angles $\phi_1 = 80(6)^\circ$ and $\phi_2 = -175(1)^\circ$) conformers, with a relative abundance of 68(8) and 32%, respectively. The differences in the structural parameters between TT and TG conformers were assumed at the *ab initio* values.

The parameters for the TT conformer are listed.

The nozzle temperature was 25 °C.



^{a)} Three times the estimated standard errors including the experimental scale error.

^{b)} Dihedral angle C(4)-N-C(2)-C(3) defined as zero for the *syn* position.

^{c)} Dihedral angle C(2)-N-C(4)-C(5) defined as zero for the *syn* position.

Kuze, N., Takeuchi, H., Egawa, T., Konaka, S., Newton, S.Q., Schäfer, L.: J. Mol. Struct. **291** (1993) 11.